Some Synchrotron Radiation Source and X-Ray Optics Simulation Software and Activities

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Collaboration Meeting on "Simulation and Modeling for SR Sources and X-Ray Optics"

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U.S. DEPARTMENT OF ENERGY | Office of Science

BROOKHAVEN NATIONAL LABORATORY | National Synchrotron Light Source II

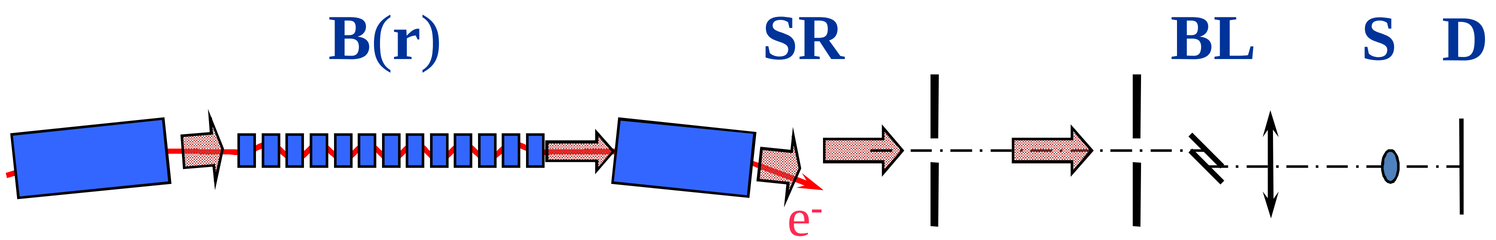
Goals of SR Source and X-Ray Optics Software Developments and Simulations

- Enable **comparison of real performances of X-ray beamlines** at NSLS-II (and other facilities) **with simulations**, determining and eliminating factors limiting the performances;
- Help in **designing** critical **diagnostics for** characterizing **electron and photon beams and X-ray optics**;
- Allow for **"start-to-end" simulation of experiments** at NSLS-II and other storage ring and FEL sources;
- Help in **development** of **new experimental techniques** and **data processing algorithms**;
- Ensure optimal **design of new beamlines** at NSLS-II and other light source facilities;
- Facilitate **creation of new** types of **X-ray optical elements**;
- Facilitate **creation of new X-ray sources**.

Connections / value to NSLS-II beamlines

- After initial commissioning, most of NSLS-II beamlines still don't show their maximal performance. The only possibility to identify losses of performance and find best strategy for "curing" them is to perform detailed comparison of the commissioning data with accurate emission and propagation simulations.
- After the real performance characteristics of beamlines are known, it may be possible to proceed to simulations of experiments, making conclusions about feasibility, required beam time, etc. This is particularly relevant to coherent scattering and microscopy type experiments (e.g. at CHX, HXN, SRX, CSX beamlines).
- Elements of the forward-simulations can be used for development of data processing algorithms for such experimental techniques as coherent scattering, coherent diffraction imaging, phase retrieval, ptychography and others, that are planned to be used at existing and future beamlines of NSLS-II.
- Simulations greatly help in development of new types of X-ray optics at NSLS-II (kinoforms, MLLs, special zone plates, bimorph and other adjustable mirrors).
- Simulations will help to identify optimal evolution path for NSLS-II, i.e. clarify benefits of further fine-tuning of the existing magnet lattice, adding more damping wigglers, etc.

Achievements: electrodynamics simulation codes for light sources (supported by NSLS-II)



- Computation of **magnetic fields** produced by permanent magnets, coils and iron blocks in 3d space, optimized for the design of **accelerator magnets**, **undulators** and **wigglers**
- Fast computation of **synchrotron radiation** emitted by relativistic electrons in magnetic fields of arbitrary configuration
- Simulation of **SR wavefront propagation** through a beamline, from source to sample
- Simulation of some **experiments** involving **SR**

RADIA code
- out of scope of this review, however very important for the development of SR sources

SRW code
- in the scope of this review

Features of some free SR source and X-ray optics simulation codes from different labs

Features \ Codes	SPECTRA	WAVE	GENESIS	SHADOW	RAY	PHASE	SRW
Source Simulation	Y	Y	Y	~Y	~N	~N	Y
Gaussian Beams	Y	Y	Y	Y	Y	~Y	Y
Spontaneous SR	Y	Y	~N	~Y (BM?)	~N	N	Y
Single-Electron	Y	Y	~N	N	~N	N	Y
Incoherent “Multi-Electron”	Y	~Y	~N	~Y (BM?)	~N	N	Y
CSR	~Y	~Y	~N	N	~N	N	~Y
SASE	N	N	Y	N	~N	N	~N
Geometrical Ray-Tracing	N	N	N	Y	Y	N	N
Wavefront Propagation	~N	N	~N	N	~N	Y	Y
Fully-Coherent Beams						Y	Y
Partially-Coherent Beams						~N	Y
Time-/Frequency-Dependent						~Y	Y
Optical Elements	N	N	N	Y	Y	Y	Y
Grazing-Incidence Mirrors				Y	Y	Y	Y
Refractive Optics				Y	Y	Y	Y
Diffractive Optics				~N	Y	~Y	Y
Gratings				Y	Y	Y	Y
Crystals				Y	Y	~N	Y
Framework	Y	Y	Y	Y	Y	Y	Y
Scripting Environment	~N	~N	~N	~Y	~N	~N	Y
File Input-Output	Y	Y	Y	Y	Y	Y	~Y
GUI	Y	Y	~N	~Y	Y	Y	~Y
Web Interface	N	N	N	N	N	N	N
API	~N	~N	~N	N	~N	~N	Y
Cross-Platform	~N	~Y	Y	Y	Y	Y	Y
Open Source	~N	~N	Y	Y	~N	N	Y
Development Effort (FTE years to date)	?	?	~4(?)	~5(?)	?	~3(?)	~5

Evolution and current status of "Synchrotron Radiation Workshop" code

- First official version of SRW was developed at ESRF in 1997-98 (written in C++, interfaced to IGOR Pro); compiled versions are distributed from: http://www.esrf.eu/Accelerators/Groups/InsertionDevices/Software/SRW
- SRW was released to Open Source in 2012 under BSD type license. To make the release possible, permissions were obtained from all previously contributed Institutes: ESRF, European XFEL, SOLEIL, DIAMOND, BNL, and from US DOE.

  The main Open Source repository, containing all C/C++ sources, C API, all interfaces and project development files, is on GitHub: https://github.com/ochubar/SRW
- SRW for Python (2.7.x and 3.x, 32- and 64-bit) cross-platform versions were released in 2012.